What is claimed is:

1. A method of simulating multibody dynamics of a molecular system so as to produce output data representative of a time evolution of the molecular system, comprising:

providing a set of equations for characterizing multibody dynamics of the molecular system, the set of equations being constrained by a constraining equation;

providing an integrator for integrating the set of equations, wherein the integrator is tailored for the set of equations so as to satisfy the constraining equation; and,

applying the integrator to the set of equations over a time step, so as to produce output data representative of the time evolution of the molecular system relative to the time step.

2. A method according to claim 1, further including applying the integrator to the set of equations over a predetermined number of time steps, so as to produce output data representative of a time evolution of the molecular system relative to a time interval corresponding to the predetermined number of time steps.

3. A method according to claim 1, wherein the constraining equation includes $|e|=1$.

4. A method according to claim 1, wherein the set of equations for characterizing multibody dynamics includes equations of motion for each of a plurality of bodies in the system, the equations of motion given by

$$\dot{e} = W(\omega)\, e$$
$$\dot{x} = C(e)u$$
$$\dot{\xi} = U_{\xi}$$
$$\dot{p}_{\omega} = G_{\omega}(q) + p^{T}\left[A_{\omega}\right]p$$
$$\dot{p}_{u} = G_{u}(q) + p^{T}\left[A_{u}\right]p$$
$$\dot{p}_{\xi} = G_{\xi}(q) + p^{T}\left[A_{\xi}\right]p$$

wherein the matrices $W(\omega)$ and $C(e)$ represent the kinematical relations and are written in the form

$$W(\omega) = \frac{1}{2}\begin{bmatrix} 0 & -\omega_x & -\omega_y & -\omega_z \\ \omega_x & 0 & \omega_z & -\omega_y \\ \omega_y & -\omega_z & 0 & \omega_x \\ \omega_z & -\omega_y & -\omega_x & 0 \end{bmatrix} \text{ and,}$$

$$C(e) = \begin{bmatrix} 1-2\left(e_2^2+e_3^2\right) & 2(e_1e_2+e_3e_0) & 2(e_1e_3-e_2e_0) \\ 2(e_2e_1-e_3e_0) & 1-2\left(e_3^2+e_1^2\right) & 2(e_2e_3+e_1e_0) \\ 2(e_3e_1+e_2e_0) & 2(e_3e_2-e_1e_0) & 1-2\left(e_1^2+e_2^2\right) \end{bmatrix}, \text{ respectively.}$$

5. A method according to claim 1, wherein applying the integrator to the set of equations over a time step further includes propagating Euler parameters of the set of equations for characterizing multibody dynamics, according to the matrix exponential of $e_{1/2} = E\left(\omega_{1/2}\right)e_0$.

6. A method according to claim 1, wherein applying the integrator to the set of equations over a time step further includes:

propagating a momentum vector to a half step $t = \Delta t/2$, while freezing one or more position states at $t = 0$;

propagating a vector of rigid position variables to the half step $t = \Delta t/2$, while freezing one or more flexible position variables at $t = 0$, and the momentum vector at $t = \Delta t/2$;

propagating the vector of flexible position variables to the full step $t = \Delta t$ using momenta, recomputed in modal velocities, at $t = \Delta t/2$:

propagating the vector of rigid position variables to the full step $t = \Delta t$, while freezing the flexible position variables at $t = \Delta t$ and the momentum vector at $t = \Delta t/2$; and,

propagating the momentum vector to the full step $t = \Delta t$ freezing the position states at $t = \Delta t$.

7. A method according to claim 1, wherein applying the integrator to the set of equations over a time step further includes decomposing the set of equations for characterizing multibody dynamics first with respect to momentum states, and then with respect to position and rigid and flexible degrees of freedom.

8. A method according to claim 1, wherein applying the integrator to the set of equations over a time step further includes decomposing the set of equations for characterizing multibody dynamics first with respect to rigid and flexible degrees of freedom, and then with respect to position and momentum states.

9. A method according to claim 1, wherein providing an integrator includes solving a kinematic equation associated with the set of equations for characterizing multibody dynamics via a solution based on a matrix exponential of the form

$$E(\omega_{1/2}) = \mathbf{e}^{W(\omega_{1/2})\frac{\Delta t}{2}} = \cos(\gamma \Delta t) I + \sin(\gamma \Delta t) D .$$

10. A computer system for simulating multibody dynamics of a molecular system so as to produce output data representative of a time evolution of the molecular system, comprising:

an analytical structure for characterizing multibody dynamics of the molecular system, wherein the analytical structure is constrained by a constraining equation;

an integrator for integrating the analytical structure, wherein the integrator is tailored for the structure so as to satisfy the constraining equation;

wherein the integrator integrates the structure over a time step, so as to produce output data representative of a time evolution of the molecular system relative to the time step.

11. A computer system according to claim 10, wherein the analytical structure includes a set of equations modeled in a computer code.

12. A computer system according to claim 11, wherein the set of equations includes equations of motion for each of a plurality of bodies in the molecular system, the equations of motion given by

$$\dot{e} = W(\omega)\, e$$
$$\dot{x} = C(e)u$$
$$\dot{\xi} = U_{\xi}$$
$$\dot{p}_{\omega} = G_{\omega}(q) + p^{T}[A_{\omega}]p$$
$$\dot{p}_{u} = G_{u}(q) + p^{T}[A_{u}]p$$
$$\dot{p}_{\xi} = G_{\xi}(q) + p^{T}[A_{\xi}]p$$

wherein the matrices $W(\omega)$ and $C(e)$ represent the kinematical relations and are written in the form

$$W(\omega) = \frac{1}{2}\begin{bmatrix} 0 & -\omega_x & -\omega_y & -\omega_z \\ \omega_x & 0 & \omega_z & -\omega_y \\ \omega_y & -\omega_z & 0 & \omega_x \\ \omega_z & -\omega_y & -\omega_x & 0 \end{bmatrix} \text{ and,}$$

$$C(e) = \begin{bmatrix} 1-2\left(e_2^2+e_3^2\right) & 2(e_1e_2+e_3e_0) & 2(e_1e_3-e_2e_0) \\ 2(e_2e_1-e_3e_0) & 1-2\left(e_3^2+e_1^2\right) & 2(e_2e_3+e_1e_0) \\ 2(e_3e_1+e_2e_0) & 2(e_3e_2-e_1e_0) & 1-2\left(e_1^2+e_2^2\right) \end{bmatrix}, \text{ respectively.}$$

13. A computer system according to claim 10, wherein the constraining equation includes $|e|=1$.

14. A computer system according to claim 10, wherein the integrator further integrates the structure over a predetermined number of time step, so as to produce output data representative of a time evolution of the molecular system relative to a time interval corresponding to the predetermined number of time steps.

15. A computer system according to claim 10, wherein the integrator further propagates Euler parameters of the set of equations for characterizing multibody dynamics, according to the matrix exponential of $e_{1/2} = E(\omega_{1/2})\, e_0$.

16. A computer system according to claim 10, wherein the integrator further solves a kinematic equation associated with the set of equations for characterizing multibody dynamics via a solution based on a matrix exponential of the form

$$E(\omega_{1/2}) = \mathbf{e}^{W(\omega_{1/2})\frac{\Delta t}{2}} = \cos(\gamma \Delta t) I + \sin(\gamma \Delta t) D.$$

17. A computer system according to claim 10, wherein the integrator further decomposes the set of equations for characterizing multibody dynamics first with respect to momentum states, and then with respect to position and rigid and flexible degrees of freedom.

18. A computer system according to claim 10, wherein the integrator further decomposes the set of equations for characterizing multibody dynamics first with respect to rigid and flexible degrees of freedom, and then with respect to position and momentum states.

19. A computer system for simulating multibody dynamics of a molecular system so as to produce output data representative of a time evolution of the molecular system, comprising:

means for characterizing multibody dynamics of the molecular system, wherein the analytical structure is constrained by a constraining equation;

means for integrating the analytical structure, wherein the integrator is tailored for the structure so as to satisfy the constraining equation;

wherein the means for integrating integrates the structure over a time step, so as to produce output data representative of a time evolution of the molecular system relative to the time step.

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20. A computer system according to claim 19, wherein the analytical structure includes equations of motion, modeled in computer code, for each of a plurality of bodies in the molecular system, the equations of motion given by

$$\dot{e} = W(\omega)\, e$$
$$\dot{x} = C(e)u$$
$$\dot{\xi} = U_{\xi}$$
$$\dot{p}_{\omega} = G_{\omega}(q) + p^{T}[A_{\omega}]p$$
$$\dot{p}_{u} = G_{u}(q) + p^{T}[A_{u}]p$$
$$\dot{p}_{\xi} = G_{\xi}(q) + p^{T}[A_{\xi}]p$$

wherein the matrices $W(\omega)$ and $C(e)$ represent the kinematical relations and are written in the form

$$W(\omega) = \frac{1}{2}\begin{bmatrix} 0 & -\omega_x & -\omega_y & -\omega_z \\ \omega_x & 0 & \omega_z & -\omega_y \\ \omega_y & -\omega_z & 0 & \omega_x \\ \omega_z & -\omega_y & -\omega_x & 0 \end{bmatrix} \text{ and,}$$

$$C(e) = \begin{bmatrix} 1-2\left(e_2^2+e_3^2\right) & 2(e_1e_2+e_3e_0) & 2(e_1e_3-e_2e_0) \\ 2(e_2e_1-e_3e_0) & 1-2\left(e_3^2+e_1^2\right) & 2(e_2e_3+e_1e_0) \\ 2(e_3e_1+e_2e_0) & 2(e_3e_2-e_1e_0) & 1-2\left(e_1^2+e_2^2\right) \end{bmatrix}, \text{ respectively.}$$